Ultrafast Light-Driven Nanomotors Based on an Acridane Stator

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# 1. SUBMISSION DETAILS

_publ_contact_author_name           # Name  of author for correspondence
;
   Drs. A. Meetsma
;
_publ_contact_author_address        # Address of author for correspondence
;
     Crystal Structure Center,
     Chemical Physics,
     Materials Science Center,
     University of Groningen,
     Nijenborgh 4,
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     The Netherlands.
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_publ_contact_author_email           A.Meetsma@rug.nl
_publ_contact_author_fax             '+31 50 3634441'
_publ_contact_author_phone           '+31 50 3634368'

_publ_requested_journal              'Journal of Organic Chemistry'
# Publication choise FI, CI or EI for Inorganic
#                    FM, CM or EM for Metal-organic
#                    FO, CO or EO for Organic
_publ_requested_category             ?
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_publ_contact_letter                # Include date of submission
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 Date of submission :  2009-09-14  12:09:23

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     Journal of Organic Chemistry

(Our Compound_Identification_Code : Q1141)
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;   # author related footnote
;
;   # Address of this author
```

```
;
   'Meetsma, Auke'
;
 ? # author related footnote
;
;
     Crystal Structure Center,
     Chemical Physics,
     Materials Science Center,
     University of Groningen,
     Nijenborgh 4,
     NL-9747 AG Groningen,
     The Netherlands.
;

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Allen, F. H. (2000). <i>Acta Cryst.</i> B<b>58</b>, 380--388.

Bondi, A. (1964). <i>J. Phys. Chem.</i> <b>68</b>, 441--451.

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Manual Bruker AXS Inc. Madison, Wisconsin, USA.

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Caro, L., Giacovazzo, C., Polidori, G. & Spagna, R. (2005). <i>SIR2004</i>. An
improved tool for crystal structure determination and refinement. J. Appl.
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```

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Spek, A. L. (2003). J. Appl. Cryst. 36, 7--13.

Wilson, A. J. C. (1992). International Tables for Crystallography, Volume C, Kluwer Academic Publishers, Dordrecht, The Netherlands.
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Fig. 1. Perspective PLUTO drawing of the molecule illustrating the configuration and the adopted numbering scheme.

Fig. 2. Molecular packing viewed down unit cell axes.

Fig. 3. Perspective ORTEP drawing of the title compound. Displacement ellipsoids for non-H are represented at the 50% probability level. The H-atoms have been omitted to improve clarity.
;

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5. CHEMICAL DATA

_chemical_name_systematic
;
;
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_chemical_melting_point   ?
_chemical_formula_moiety
'C33 H31 N O3'
Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'
_chemical_formula_structural   ?
_chemical_formula_sum
'C33 H31 N O3'
_chemical_formula_iupac   ?
_chemical_formula_weight   489.61
_chemical_compound_source   'see text'

loop_
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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
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# 6. CRYSTAL DATA

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loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
   1 x,y,z
   2 -x,1/2+y,1/2-z
   3 -x,-y,-z
   4 x,1/2-y,1/2+z

_cell_length_a                        9.020(2)
_cell_length_b                       18.831(3)
_cell_length_c                       30.265(5)
_cell_angle_alpha                    90
_cell_angle_beta                     95.108(3)
_cell_angle_gamma                    90
_cell_volume                       5120.3(16)
_cell_formula_units_Z               8

_cell_measurement_temperature    100(1)
_cell_measurement_reflns_used      5340
_cell_measurement_theta_min        2.51
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_cell_special_details
;
 The final unit cell was obtained from the xyz centroids of
   5340 reflections after integration using the SAINTPLUS
   software package (Bruker, 2000).

 Reduced cell calculations did not indicate any higher metric lattice symmetry
   and examination of the finalatomic coordinates of the structure did not
   yield extra symmetry elements (Spek, 1988; Le Page 1987, 1988)
;

_exptl_crystal_description       'needle'
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_exptl_crystal_size_min           0.035
_exptl_crystal_size_rad           ?
_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     1.270
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_exptl_crystal_F_000              2080
_exptl_absorpt_coefficient_mu     0.081
_exptl_absorpt_correction_type    'Multi-Scan'
_exptl_absorpt_process_details    '(SADABS, Sheldrick, Bruker, 2001))'
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_exptl_absorpt_correction_T_min    0.9665
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# 7. EXPERIMENTAL DATA

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_diffrn_radiation_type                'MoK\a'
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_diffrn_radiation_monochromator       'parallel mounted graphite'
_diffrn_radiation_detector
;
  CCD area-detector
;
_diffrn_measurement_device_type
;
  Bruker Smart Apex; CCD area detector
;
_diffrn_measurement_method            '\f and \w scans'
_diffrn_special_details
;
 Crystal into the cold nitrogen stream of the low-temparature unit
   (KRYOFLEX, (Bruker, 2000)).
;
_diffrn_detector_area_resol_mean      66.06

_diffrn_standards_number              0
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_diffrn_standards_decay_%             0

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_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
 ? ? ?

# number of measured reflections (redundant set)
_diffrn_reflns_number              39203
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_diffrn_reflns_av_sigmaI/netI      0.0834
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_diffrn_reflns_limit_k_min         -23
_diffrn_reflns_limit_k_max         23
_diffrn_reflns_limit_l_min         -37
_diffrn_reflns_limit_l_max         37
_diffrn_reflns_theta_min           2.55
_diffrn_reflns_theta_max           26.02
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_diffrn_reflns_theta_full              25.00
_diffrn_measured_fraction_theta_full   0.995

_diffrn_reflns_reduction_process
;
 Intensity data were corrected for Lorentz and polarization
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  effects, decay and absorption and reduced to F~o~^2^
  using SAINT (Bruker, 2000) and SADABS (Sheldrick, 2001)
;

# number of unique reflections
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_reflns_number_gt                 6490
_reflns_threshold_expression     I>2\s(I)


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_computing_cell_refinement          'SAINTPLUS, Version 6.02A, (Bruker, 2001)'
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_computing_structure_solution
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 SIR2004 (Burla et al., 2005)
;
_computing_structure_refinement      'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
 PLUTO (Meetsma, 2006)
 PLATON (Spek, 2003)
;
_computing_publication_material      'PLATON (Spek, 2003)'

#===============================================================================

# 8. REFINEMENT DATA


_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_matrix_type           full
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_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0506P)^2^+0.1669P] where P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary   direct
_atom_sites_solution_hydrogens   difmap
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_refine_ls_extinction_method     none
_refine_ls_extinction_coef       ?
_refine_ls_abs_structure_details  ?
_chemical_absolute_configuration  '.'

_refine_ls_abs_structure_Flack   ?
_refine_ls_number_reflns         10011
_refine_ls_number_parameters     915
_refine_ls_number_restraints     0
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_refine_ls_R_factor_all          0.0938
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_refine_ls_restrained_S_all       1.009
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_refine_ls_shift/su_mean          0.000

_refine_diff_density_max          0.212
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O12 O Uani 0.40750(15) 0.15907(7) 0.53386(4) 1.000 0.0157(5) . .
O13 O Uani -0.11514(16) 0.33340(7) 0.59494(4) 1.000 0.0192(5) . .
N11 N Uani 0.18207(18) 0.13130(8) 0.50154(5) 1.000 0.0139(5) . .
C11 C Uani 0.0831(2) 0.10080(11) 0.46692(6) 1.000 0.0150(7) . .
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C13 C Uani -0.0206(3) 0.00102(12) 0.42639(7) 1.000 0.0219(7) . .
C14 C Uani -0.1303(3) 0.04406(12) 0.40573(7) 1.000 0.0213(7) . .
C15 C Uani -0.1310(3) 0.11582(11) 0.41467(7) 1.000 0.0180(7) . .
C16 C Uani -0.0217(2) 0.14636(11) 0.44432(6) 1.000 0.0156(7) . .
C17 C Uani -0.0080(2) 0.22323(11) 0.45605(6) 1.000 0.0139(6) . .
C18 C Uani 0.0171(2) 0.23148(10) 0.50469(6) 1.000 0.0130(7) . .
C19 C Uani -0.0590(2) 0.28048(11) 0.52868(7) 1.000 0.0130(6) . .
C110 C Uani -0.0331(2) 0.28392(10) 0.57430(7) 1.000 0.0151(7) . .
C111 C Uani 0.0691(2) 0.23820(11) 0.59690(7) 1.000 0.0164(7) . .
C112 C Uani 0.1409(2) 0.18778(11) 0.57316(7) 1.000 0.0157(7) . .
C113 C Uani 0.1158(2) 0.18435(10) 0.52746(6) 1.000 0.0135(6) . .
C114 C Uani 0.3315(2) 0.11303(11) 0.50652(6) 1.000 0.0144(6) . .
C115 C Uani 0.5622(2) 0.14242(11) 0.55206(7) 1.000 0.0173(7) . .
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C117 C Uani 0.5582(3) 0.07600(12) 0.58012(8) 1.000 0.0221(8) . .
C118 C Uani 0.6015(3) 0.20729(12) 0.58023(8) 1.000 0.0222(8) . .
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C130 C Uani 0.2307(2) 0.35469(12) 0.49736(7) 1.000 0.0169(7) . .
C131 C Uani 0.1266(2) 0.38857(10) 0.46663(6) 1.000 0.0144(7) . .
C132 C Uani 0.0277(2) 0.35316(10) 0.43398(6) 1.000 0.0140(6) . .
C133 C Uani 0.0683(3) 0.25028(14) 0.34974(8) 1.000 0.0239(8) . .


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H19 H Uiso -0.133(2) 0.3125(10) 0.5138(6) 1.000 0.009(5) . .
H111 H Uiso 0.090(2) 0.2419(11) 0.6293(7) 1.000 0.023(6) . .
H112 H Uiso 0.206(2) 0.1557(10) 0.5888(6) 1.000 0.013(5) . .
H116 H Uiso 0.650(3) 0.0907(13) 0.4975(8) 1.000 0.034(7) . .
H116' H Uiso 0.768(3) 0.1344(11) 0.5295(7) 1.000 0.021(6) . .
H116" H Uiso 0.657(2) 0.1771(12) 0.4965(7) 1.000 0.022(6) . .
H117 H Uiso 0.491(3) 0.0823(12) 0.6033(8) 1.000 0.031(6) . .
H117' H Uiso 0.662(3) 0.0658(12) 0.5944(8) 1.000 0.037(7) . .
H117" H Uiso 0.532(2) 0.0333(12) 0.5628(7) 1.000 0.023(6) . .
H118 H Uiso 0.602(2) 0.2504(12) 0.5616(7) 1.000 0.028(6) . .
H118' H Uiso 0.703(3) 0.2002(12) 0.5963(7) 1.000 0.032(7) . .
H118" H Uiso 0.526(3) 0.2155(12) 0.6038(8) 1.000 0.032(6) . .
H119 H Uiso -0.089(3) 0.3053(13) 0.6591(8) 1.000 0.034(7) . .
H119' H Uiso -0.130(3) 0.3942(14) 0.6483(8) 1.000 0.048(7) . .
H119" H Uiso 0.042(3) 0.3624(13) 0.6442(8) 1.000 0.041(8) . .
H121 H Uiso -0.143(2) 0.2341(10) 0.3707(6) 1.000 0.017(5) . .
H122 H Uiso -0.102(2) 0.3577(11) 0.3347(8) 1.000 0.025(6) . .
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H125 H Uiso 0.040(2) 0.5536(11) 0.4338(6) 1.000 0.015(5) . .
H127 H Uiso 0.228(3) 0.5563(13) 0.4950(7) 1.000 0.035(7) . .
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H130 H Uiso 0.236(2) 0.3039(12) 0.4972(7) 1.000 0.022(6) . .
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O21 O Uani 0.81625(16) 0.51495(7) 0.29313(5) 1.000 0.0216(5) . .
O22 O Uani 0.79031(16) 0.42704(8) 0.24187(5) 1.000 0.0232(5) . .
O23 O Uani 0.24959(17) 0.23469(8) 0.20242(4) 1.000 0.0232(5) . .
N21 N Uani 0.59770(19) 0.45320(9) 0.28111(5) 1.000 0.0165(5) . .
C21 C Uani 0.5328(2) 0.48495(11) 0.31836(6) 1.000 0.0159(7) . .
C22 C Uani 0.5394(3) 0.55737(11) 0.32531(7) 1.000 0.0186(7) . .
C23 C Uani 0.4678(3) 0.58684(12) 0.35940(7) 1.000 0.0223(8) . .
C24 C Uani 0.3873(3) 0.54440(12) 0.38565(7) 1.000 0.0198(7) . .
C25 C Uani 0.3794(2) 0.47205(11) 0.37858(7) 1.000 0.0171(7) . .
C26 C Uani 0.4558(2) 0.44023(10) 0.34556(6) 1.000 0.0146(7) . .
C27 C Uani 0.4587(2) 0.36319(10) 0.33520(6) 1.000 0.0134(6) . .
C28 C Uani 0.4408(2) 0.35177(10) 0.28681(6) 1.000 0.0143(6) . .
C29 C Uani 0.3485(2) 0.29816(11) 0.26800(7) 1.000 0.0158(7) . .
C210 C Uani 0.3324(2) 0.28856(11) 0.22288(7) 1.000 0.0174(7) . .
C211 C Uani 0.4044(3) 0.33404(12) 0.19566(7) 1.000 0.0195(7) . .
C212 C Uani 0.4920(3) 0.38872(12) 0.21365(7) 1.000 0.0196(7) . .
C213 C Uani 0.5115(2) 0.39710(10) 0.25942(6) 1.000 0.0146(7) . .
```

```
C214 C Uani 0.7433(2) 0.46927(11) 0.27354(7) 1.000 0.0176(7) . .
C215 C Uani 0.9338(3) 0.44277(12) 0.22291(7) 1.000 0.0243(8) . .
C216 C Uani 1.0633(3) 0.43578(15) 0.25794(9) 1.000 0.0316(9) . .
C217 C Uani 0.9246(3) 0.51538(14) 0.20142(9) 1.000 0.0324(9) . .
C218 C Uani 0.9385(4) 0.38475(17) 0.18830(11) 1.000 0.0419(11) . .
C219 C Uani 0.1945(3) 0.18258(13) 0.23111(8) 1.000 0.0242(8) . .
C220 C Uani 0.4783(2) 0.30884(11) 0.36469(6) 1.000 0.0132(6) . .
C221 C Uani 0.4606(2) 0.31291(11) 0.41428(6) 1.000 0.0151(7) . .
C222 C Uani 0.3994(3) 0.23875(11) 0.42453(7) 1.000 0.0172(7) . .
C223 C Uani 0.4500(2) 0.19268(11) 0.38855(7) 1.000 0.0156(6) . .
C224 C Uani 0.4458(3) 0.11804(11) 0.38643(7) 1.000 0.0201(7) . .
C225 C Uani 0.5017(3) 0.08494(12) 0.35149(7) 1.000 0.0220(7) . .
C226 C Uani 0.5733(2) 0.12308(11) 0.31891(7) 1.000 0.0173(7) . .
C227 C Uani 0.6428(3) 0.08721(12) 0.28548(7) 1.000 0.0228(7) . .
C228 C Uani 0.7211(3) 0.12305(12) 0.25614(7) 1.000 0.0238(8) . .
C229 C Uani 0.7341(2) 0.19705(12) 0.25934(7) 1.000 0.0195(7) . .
C230 C Uani 0.6654(2) 0.23372(11) 0.29076(7) 1.000 0.0158(7) . .
C231 C Uani 0.5791(2) 0.19844(11) 0.32114(6) 1.000 0.0147(6) . .
C232 C Uani 0.5045(2) 0.23278(11) 0.35522(6) 1.000 0.0142(6) . .
C233 C Uani 0.6067(3) 0.32838(13) 0.44204(7) 1.000 0.0204(7) . .


H22 H Uiso 0.589(2) 0.5862(11) 0.3052(7) 1.000 0.016(5) . .
H23 H Uiso 0.467(2) 0.6392(12) 0.3636(7) 1.000 0.028(6) . .
H24 H Uiso 0.338(2) 0.5658(10) 0.4095(6) 1.000 0.013(5) . .
H25 H Uiso 0.319(2) 0.4446(10) 0.3967(7) 1.000 0.014(5) . .
H29 H Uiso 0.301(2) 0.2705(11) 0.2864(7) 1.000 0.020(6) . .
H211 H Uiso 0.390(2) 0.3266(10) 0.1646(7) 1.000 0.014(5) . .
H212 H Uiso 0.545(2) 0.4190(11) 0.1951(7) 1.000 0.022(6) . .
H216 H Uiso 1.066(3) 0.4730(13) 0.2815(8) 1.000 0.037(7) . .
H216' H Uiso 1.157(3) 0.4391(12) 0.2438(8) 1.000 0.035(7) . .
H216" H Uiso 1.065(3) 0.3866(15) 0.2739(9) 1.000 0.056(8) . .
H217 H Uiso 0.838(3) 0.5173(12) 0.1792(8) 1.000 0.036(7) . .
H217' H Uiso 1.016(2) 0.5242(11) 0.1866(7) 1.000 0.024(6) . .
H217" H Uiso 0.927(3) 0.5542(14) 0.2261(9) 1.000 0.054(8) . .
H218 H Uiso 0.942(3) 0.3380(14) 0.2026(8) 1.000 0.040(8) . .
H218' H Uiso 1.033(3) 0.3903(13) 0.1723(8) 1.000 0.046(7) . .
H218" H Uiso 0.853(4) 0.3859(18) 0.1671(11) 1.000 0.087(13) . .
H219 H Uiso 0.280(3) 0.1646(13) 0.2530(8) 1.000 0.040(7) . .
H219' H Uiso 0.155(2) 0.1410(12) 0.2113(7) 1.000 0.027(6) . .
H219" H Uiso 0.110(3) 0.2036(11) 0.2482(7) 1.000 0.027(6) . .
H221 H Uiso 0.388(2) 0.3485(11) 0.4204(7) 1.000 0.020(6) . .
H222 H Uiso 0.439(2) 0.2223(10) 0.4547(7) 1.000 0.015(5) . .
H222' H Uiso 0.287(2) 0.2384(10) 0.4240(6) 1.000 0.017(5) . .
H224 H Uiso 0.400(2) 0.0910(10) 0.4102(7) 1.000 0.013(5) . .
H225 H Uiso 0.497(2) 0.0325(12) 0.3501(7) 1.000 0.021(6) . .
H227 H Uiso 0.636(2) 0.0352(12) 0.2842(7) 1.000 0.028(6) . .
H228 H Uiso 0.767(2) 0.0951(12) 0.2319(7) 1.000 0.031(6) . .
H229 H Uiso 0.794(2) 0.2218(11) 0.2385(7) 1.000 0.018(5) . .
H230 H Uiso 0.676(2) 0.2847(10) 0.2934(6) 1.000 0.009(5) . .
H233 H Uiso 0.684(3) 0.2895(12) 0.4379(7) 1.000 0.031(6) . .
H233' H Uiso 0.588(2) 0.3321(11) 0.4748(7) 1.000 0.021(6) . .
H233" H Uiso 0.649(3) 0.3738(13) 0.4343(7) 1.000 0.032(7) . .


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O11 0.0204(9) 0.0206(8) 0.0198(8) -0.0034(7) 0.0025(7) 0.0059(7)
O12 0.0122(8) 0.0173(8) 0.0174(8) -0.0008(6) -0.0002(6) 0.0009(6)
O13 0.0234(9) 0.0206(8) 0.0140(8) -0.0037(6) 0.0036(7) 0.0062(7)
N11 0.0133(10) 0.0148(9) 0.0136(9) -0.0022(7) 0.0006(8) 0.0026(7)
C11 0.0149(12) 0.0195(11) 0.0112(11) -0.0024(9) 0.0040(9) -0.0024(9)
C12 0.0216(13) 0.0176(12) 0.0157(12) -0.0008(9) 0.0049(10) 0.0007(10)
C13 0.0290(14) 0.0167(12) 0.0210(12) -0.0037(10) 0.0077(11) -0.0034(10)
C14 0.0202(13) 0.0253(13) 0.0179(12) -0.0054(10) -0.0013(10) -0.0045(10)
C15 0.0171(13) 0.0198(12) 0.0173(12) -0.0016(9) 0.0021(10) -0.0005(10)
C16 0.0158(12) 0.0201(11) 0.0115(11) -0.0005(9) 0.0044(9) -0.0004(9)
C17 0.0084(11) 0.0197(11) 0.0137(11) -0.0027(9) 0.0009(9) 0.0009(9)
C18 0.0128(12) 0.0130(11) 0.0132(11) 0.0004(8) 0.0011(9) -0.0035(9)
C19 0.0099(11) 0.0136(11) 0.0153(11) 0.0034(9) 0.0008(9) -0.0005(9)
C110 0.0166(12) 0.0115(10) 0.0177(12) -0.0020(9) 0.0038(9) -0.0011(9)
C111 0.0196(13) 0.0179(11) 0.0120(11) 0.0003(9) 0.0031(9) -0.0022(9)
C112 0.0137(12) 0.0163(11) 0.0168(12) 0.0043(9) 0.0000(9) 0.0004(9)
C113 0.0131(11) 0.0137(11) 0.0142(11) -0.0016(8) 0.0037(9) -0.0017(9)
C114 0.0182(12) 0.0143(11) 0.0105(10) 0.0022(9) 0.0004(9) 0.0002(9)
C115 0.0104(12) 0.0218(12) 0.0194(12) 0.0019(9) 0.0000(9) 0.0018(9)
C116 0.0161(14) 0.0246(14) 0.0259(13) 0.0033(11) 0.0046(11) 0.0030(10)
C117 0.0242(15) 0.0213(13) 0.0207(13) 0.0021(10) 0.0011(11) 0.0018(11)
C118 0.0190(14) 0.0204(13) 0.0271(14) -0.0028(10) 0.0015(12) -0.0021(10)
C119 0.0388(17) 0.0296(14) 0.0144(12) -0.0051(11) -0.0007(11) 0.0120(12)
C120 0.0105(11) 0.0201(11) 0.0124(11) -0.0022(9) 0.0022(9) 0.0007(9)
C121 0.0162(12) 0.0208(12) 0.0119(11) -0.0007(9) -0.0007(9) -0.0038(10)
C122 0.0171(13) 0.0247(12) 0.0127(12) 0.0012(9) 0.0015(10) -0.0005(10)
C123 0.0122(12) 0.0229(12) 0.0147(11) 0.0043(9) 0.0040(9) -0.0016(9)
C124 0.0200(13) 0.0219(12) 0.0185(12) 0.0063(10) 0.0016(10) 0.0030(10)
C125 0.0244(13) 0.0134(12) 0.0270(13) 0.0029(10) 0.0063(11) 0.0018(10)
C126 0.0166(12) 0.0197(12) 0.0156(11) 0.0003(9) 0.0063(9) -0.0008(9)
C127 0.0246(14) 0.0194(13) 0.0239(13) -0.0017(10) 0.0025(10) -0.0014(10)
C128 0.0235(14) 0.0250(13) 0.0209(13) -0.0072(10) -0.0012(11) -0.0049(10)
C129 0.0193(13) 0.0247(13) 0.0179(12) -0.0002(10) -0.0008(10) -0.0006(10)
C130 0.0180(13) 0.0193(12) 0.0143(11) -0.0010(9) 0.0060(9) -0.0014(10)
C131 0.0142(12) 0.0164(11) 0.0131(11) -0.0014(9) 0.0048(9) -0.0006(9)
C132 0.0124(11) 0.0183(11) 0.0120(11) 0.0004(9) 0.0050(9) 0.0018(9)
C133 0.0247(14) 0.0364(15) 0.0103(12) -0.0027(10) -0.0004(10) 0.0053(12)
O21 0.0217(9) 0.0200(8) 0.0233(9) 0.0010(7) 0.0032(7) -0.0023(7)
O22 0.0198(9) 0.0249(9) 0.0268(9) -0.0046(7) 0.0120(7) -0.0012(7)
O23 0.0293(10) 0.0247(9) 0.0148(8) -0.0033(7) -0.0028(7) -0.0042(7)
N21 0.0180(10) 0.0161(9) 0.0159(9) -0.0009(7) 0.0050(8) -0.0012(8)
C21 0.0140(12) 0.0205(12) 0.0131(11) -0.0001(9) 0.0009(9) 0.0038(9)
C22 0.0199(13) 0.0167(12) 0.0190(12) 0.0043(9) 0.0007(10) 0.0000(9)
C23 0.0239(13) 0.0190(13) 0.0231(13) -0.0023(10) -0.0027(10) 0.0041(10)
C24 0.0207(13) 0.0245(12) 0.0141(12) -0.0039(10) 0.0007(10) 0.0063(10)
C25 0.0163(12) 0.0194(12) 0.0151(11) 0.0021(9) -0.0005(10) 0.0038(9)
C26 0.0125(12) 0.0173(11) 0.0135(11) 0.0004(9) -0.0023(9) 0.0016(9)
C27 0.0106(11) 0.0164(11) 0.0133(11) -0.0028(9) 0.0017(9) -0.0001(9)
C28 0.0134(11) 0.0150(11) 0.0148(11) 0.0011(9) 0.0032(9) 0.0048(9)
C29 0.0148(12) 0.0182(12) 0.0148(12) 0.0029(9) 0.0031(10) 0.0044(9)
C210 0.0180(12) 0.0192(12) 0.0146(11) -0.0024(9) -0.0014(9) 0.0040(9)
C211 0.0261(13) 0.0251(12) 0.0073(11) 0.0010(9) 0.0009(10) 0.0050(10)
C212 0.0229(13) 0.0228(12) 0.0138(12) 0.0029(10) 0.0055(10) 0.0026(10)
C213 0.0164(12) 0.0133(11) 0.0141(11) -0.0004(9) 0.0008(9) 0.0031(9)
C214 0.0216(13) 0.0163(12) 0.0151(11) 0.0057(9) 0.0036(10) 0.0016(10)
C215 0.0196(13) 0.0291(13) 0.0258(13) 0.0009(10) 0.0110(10) -0.0001(10)
C216 0.0220(15) 0.0371(16) 0.0369(16) 0.0070(13) 0.0087(13) 0.0069(12)
C217 0.0274(16) 0.0401(16) 0.0312(16) 0.0109(13) 0.0107(14) 0.0017(12)
C218 0.0383(19) 0.0433(19) 0.0481(19) -0.0144(15) 0.0262(16) -0.0035(15)
```

```
C219 0.0290(15) 0.0212(13) 0.0215(13) -0.0031(10) -0.0030(12) -0.0043(11)
C220 0.0077(11) 0.0188(11) 0.0130(11) 0.0003(9) 0.0008(9) -0.0009(9)
C221 0.0159(12) 0.0199(12) 0.0098(11) 0.0007(9) 0.0025(9) 0.0040(10)
C222 0.0175(13) 0.0204(12) 0.0141(12) 0.0016(9) 0.0042(10) -0.0023(10)
C223 0.0106(11) 0.0206(11) 0.0147(11) 0.0023(9) -0.0043(9) -0.0003(9)
C224 0.0224(13) 0.0201(12) 0.0174(12) 0.0050(9) 0.0001(10) -0.0036(10)
C225 0.0224(13) 0.0160(12) 0.0265(13) 0.0008(10) -0.0032(10) 0.0000(10)
C226 0.0176(12) 0.0185(12) 0.0150(11) -0.0007(9) -0.0032(9) 0.0000(9)
C227 0.0268(14) 0.0192(12) 0.0218(12) -0.0049(10) -0.0018(10) 0.0012(10)
C228 0.0252(14) 0.0271(13) 0.0191(12) -0.0056(10) 0.0020(11) 0.0065(10)
C229 0.0173(12) 0.0255(13) 0.0158(12) -0.0001(10) 0.0021(10) 0.0015(10)
C230 0.0150(12) 0.0182(12) 0.0137(11) -0.0001(9) -0.0020(9) 0.0015(9)
C231 0.0111(11) 0.0190(11) 0.0131(11) -0.0012(9) -0.0037(9) 0.0020(9)
C232 0.0101(11) 0.0190(11) 0.0129(11) 0.0004(9) -0.0016(9) 0.0003(9)
C233 0.0218(13) 0.0251(13) 0.0141(12) -0.0009(10) 0.0013(10) -0.0043(11)

#===============================================================================

# 10. MOLECULAR GEOMETRY

_geom_special_details
;
 Bond distances, angles etc. have been calculated using the
 rounded fractional coordinates. All su's are estimated
 from the variances of the (full) variance-covariance matrix.
 The cell esds are taken into account in the estimation of
 distances, angles and torsion angles
;

loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
 O11     C114       1.204(2)                    .       .                  yes
 O12     C114       1.344(2)                    .       .                  yes
 O12     C115       1.487(2)                    .       .                  yes
 O13     C110       1.374(2)                    .       .                  yes
 O13     C119       1.431(3)                    .       .                  yes
 O21     C214       1.206(2)                    .       .                  yes
 O22     C215       1.492(3)                    .       .                  yes
 O22     C214       1.343(3)                    .       .                  yes
 O23     C210       1.374(3)                    .       .                  yes
 O23     C219       1.429(3)                    .       .                  yes
 N11     C11        1.435(2)                    .       .                  yes
 N11     C114       1.386(2)                    .       .                  yes
 N11     C113       1.433(2)                    .       .                  yes
 N21     C213       1.436(3)                    .       .                  yes
 N21     C21        1.445(2)                    .       .                  yes
 N21     C214       1.387(3)                    .       .                  yes
 C11     C12        1.386(3)                    .       .                  no
 C11     C16        1.408(3)                    .       .                  no
 C12     C13        1.376(3)                    .       .                  no
 C13     C14        1.385(3)                    .       .                  no
 C14     C15        1.378(3)                    .       .                  no
 C15     C16        1.397(3)                    .       .                  no
 C16     C17        1.493(3)                    .       .                  no
 C17     C18        1.478(3)                    .       .                  no
 C17     C120       1.354(3)                    .       .                  no
```

C18	C113	1.395(3)	.	.	no
C18	C19	1.392(3)	.	.	no
C19	C110	1.381(3)	.	.	no
C110	C111	1.395(3)	.	.	no
C111	C112	1.386(3)	.	.	no
C112	C113	1.383(3)	.	.	no
C12	H12	0.942(19)	.	.	no
C13	H13	0.97(2)	.	.	no
C14	H14	0.98(2)	.	.	no
C115	C116	1.520(3)	.	.	no
C115	C118	1.514(3)	.	.	no
C15	H15	0.97(2)	.	.	no
C115	C117	1.514(3)	.	.	no
C19	H19	0.979(18)	.	.	no
C120	C132	1.481(3)	.	.	no
C120	C121	1.529(3)	.	.	no
C121	C122	1.537(3)	.	.	no
C121	C133	1.526(3)	.	.	no
C122	C123	1.495(3)	.	.	no
C123	C132	1.380(3)	.	.	no
C123	C124	1.399(3)	.	.	no
C124	C125	1.359(3)	.	.	no
C125	C126	1.418(3)	.	.	no
C126	C131	1.428(3)	.	.	no
C126	C127	1.412(3)	.	.	no
C127	C128	1.364(3)	.	.	no
C128	C129	1.393(3)	.	.	no
C129	C130	1.375(3)	.	.	no
C130	C131	1.414(3)	.	.	no
C131	C132	1.435(3)	.	.	no
C111	H111	0.98(2)	.	.	no
C112	H112	0.940(19)	.	.	no
C116	H116"	0.99(2)	.	.	no
C116	H116	1.00(2)	.	.	no
C116	H116'	0.97(3)	.	.	no
C117	H117"	0.98(2)	.	.	no
C117	H117	0.97(3)	.	.	no
C117	H117'	1.01(3)	.	.	no
C118	H118"	1.04(3)	.	.	no
C118	H118	0.99(2)	.	.	no
C118	H118'	1.01(3)	.	.	no
C119	H119'	1.07(3)	.	.	no
C119	H119"	1.01(3)	.	.	no
C119	H119	1.03(2)	.	.	no
C121	H121	1.027(18)	.	.	no
C21	C22	1.380(3)	.	.	no
C21	C26	1.404(3)	.	.	no
C22	C23	1.381(3)	.	.	no
C122	H122'	0.994(18)	.	.	no
C122	H122	0.97(2)	.	.	no
C23	C24	1.378(3)	.	.	no
C124	H124	0.94(2)	.	.	no
C24	C25	1.380(3)	.	.	no
C25	C26	1.398(3)	.	.	no
C125	H125	0.98(2)	.	.	no
C26	C27	1.485(3)	.	.	no
C127	H127	1.03(2)	.	.	no
C27	C220	1.359(3)	.	.	no
C27	C28	1.475(3)	.	.	no
C128	H128	0.93(2)	.	.	no
C28	C213	1.384(3)	.	.	no

C28	C29	1.397(3)	.	.	no
C129	H129	0.98(2)	.	.	no
C29	C210	1.372(3)	.	.	no
C130	H130	0.96(2)	.	.	no
C133	H133"	1.01(2)	.	.	no
C133	H133'	0.98(2)	.	.	no
C133	H133	1.06(3)	.	.	no
C22	H22	0.96(2)	.	.	no
C23	H23	0.99(2)	.	.	no
C24	H24	0.969(18)	.	.	no
C25	H25	0.958(19)	.	.	no
C29	H29	0.90(2)	.	.	no
C210	C211	1.389(3)	.	.	no
C211	C212	1.380(3)	.	.	no
C212	C213	1.390(3)	.	.	no
C215	C216	1.512(4)	.	.	no
C215	C217	1.513(3)	.	.	no
C215	C218	1.517(4)	.	.	no
C220	C221	1.525(3)	.	.	no
C220	C232	1.484(3)	.	.	no
C221	C222	1.543(3)	.	.	no
C221	C233	1.527(3)	.	.	no
C222	C223	1.495(3)	.	.	no
C223	C224	1.407(3)	.	.	no
C223	C232	1.385(3)	.	.	no
C224	C225	1.362(3)	.	.	no
C225	C226	1.421(3)	.	.	no
C226	C231	1.422(3)	.	.	no
C226	C227	1.409(3)	.	.	no
C227	C228	1.362(3)	.	.	no
C228	C229	1.401(3)	.	.	no
C229	C230	1.368(3)	.	.	no
C230	C231	1.421(3)	.	.	no
C231	C232	1.435(3)	.	.	no
C211	H211	0.95(2)	.	.	no
C212	H212	0.96(2)	.	.	no
C216	H216'	0.98(3)	.	.	no
C216	H216"	1.04(3)	.	.	no
C216	H216	1.00(2)	.	.	no
C217	H217'	0.987(19)	.	.	no
C217	H217"	1.04(3)	.	.	no
C217	H217	0.99(3)	.	.	no
C218	H218'	1.02(3)	.	.	no
C218	H218"	0.96(3)	.	.	no
C218	H218	0.98(3)	.	.	no
C219	H219'	1.03(2)	.	.	no
C219	H219"	1.04(3)	.	.	no
C219	H219	1.03(3)	.	.	no
C221	H221	0.97(2)	.	.	no
C222	H222'	1.013(18)	.	.	no
C222	H222	1.00(2)	.	.	no
C224	H224	1.00(2)	.	.	no
C225	H225	0.99(2)	.	.	no
C227	H227	0.98(2)	.	.	no
C228	H228	1.02(2)	.	.	no
C229	H229	0.98(2)	.	.	no
C230	H230	0.967(19)	.	.	no
C233	H233'	1.02(2)	.	.	no
C233	H233"	0.97(3)	.	.	no
C233	H233	1.03(3)	.	.	no

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 C114    O12     C115     120.16(15)              .       .       .          yes
 C110    O13     C119     116.40(17)              .       .       .          yes
 C214    O22     C215     119.80(16)              .       .       .          yes
 C210    O23     C219     115.96(16)              .       .       .          yes
 C113    N11     C114     124.22(15)              .       .       .          yes
 C11     N11     C113     114.59(15)              .       .       .          yes
 C11     N11     C114     121.05(15)              .       .       .          yes
 C21     N21     C213     114.88(15)              .       .       .          yes
 C21     N21     C214     119.61(16)              .       .       .          yes
 C213    N21     C214     124.58(16)              .       .       .          yes
 N11     C11     C12      121.78(18)              .       .       .          yes
 C12     C11     C16      120.86(18)              .       .       .          no
 N11     C11     C16      117.26(17)              .       .       .          yes
 C11     C12     C13        119.7(2)              .       .       .          no
 C12     C13     C14        120.4(2)              .       .       .          no
 C13     C14     C15        120.1(2)              .       .       .          no
 C14     C15     C16        121.0(2)              .       .       .          no
 C11     C16     C17      115.95(16)              .       .       .          no
 C15     C16     C17      126.22(18)              .       .       .          no
 C11     C16     C15      117.79(19)              .       .       .          no
 C18     C17     C120     124.88(18)              .       .       .          no
 C16     C17     C18      109.94(16)              .       .       .          no
 C16     C17     C120     125.03(17)              .       .       .          no
 C17     C18     C19      123.39(17)              .       .       .          no
 C17     C18     C113     117.37(17)              .       .       .          no
 C19     C18     C113     119.12(17)              .       .       .          no
 C18     C19     C110     120.33(18)              .       .       .          no
 C19     C110    C111     120.44(18)              .       .       .          no
 O13     C110    C111     123.68(18)              .       .       .          yes
 O13     C110    C19      115.86(17)              .       .       .          yes
 C110    C111    C112     119.18(19)              .       .       .          no
 C111    C112    C113     120.54(18)              .       .       .          no
 C11     C12     H12       117.9(12)              .       .       .          no
 C13     C12     H12       122.4(12)              .       .       .          no
 C14     C13     H13       121.1(12)              .       .       .          no
 N11     C113    C112     122.74(17)              .       .       .          yes
 C18     C113    C112     120.32(17)              .       .       .          no
 N11     C113    C18      116.87(16)              .       .       .          yes
 C12     C13     H13       118.4(12)              .       .       .          no
 O12     C114    N11      110.16(16)              .       .       .          yes
 C13     C14     H14       122.5(11)              .       .       .          no
 O11     C114    O12      125.86(17)              .       .       .          yes
 O11     C114    N11      123.96(18)              .       .       .          yes
 C15     C14     H14       117.4(11)              .       .       .          no
 C14     C15     H15       117.2(12)              .       .       .          no
 O12     C115    C116     111.81(17)              .       .       .          yes
 O12     C115    C117     108.27(16)              .       .       .          yes
 C16     C15     H15       121.7(12)              .       .       .          no
 C116    C115    C118     111.01(18)              .       .       .          no
 C117    C115    C118     111.52(18)              .       .       .          no
 O12     C115    C118     101.74(16)              .       .       .          yes
 C116    C115    C117     112.03(19)              .       .       .          no
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C18	C19	H19	121.1(11)	.	.	.	no
C110	C19	H19	118.6(11)	.	.	.	no
C17	C120	C121	124.73(18)	.	.	.	no
C121	C120	C132	105.64(16)	.	.	.	no
C17	C120	C132	129.45(17)	.	.	.	no
C120	C121	C122	103.37(16)	.	.	.	no
C120	C121	C133	111.75(16)	.	.	.	no
C122	C121	C133	111.50(18)	.	.	.	no
C121	C122	C123	104.10(18)	.	.	.	no
C124	C123	C132	122.49(19)	.	.	.	no
C122	C123	C124	126.02(19)	.	.	.	no
C122	C123	C132	111.49(18)	.	.	.	no
C123	C124	C125	118.9(2)	.	.	.	no
C124	C125	C126	121.2(2)	.	.	.	no
C127	C126	C131	119.52(18)	.	.	.	no
C125	C126	C127	120.3(2)	.	.	.	no
C125	C126	C131	120.06(18)	.	.	.	no
C126	C127	C128	121.3(2)	.	.	.	no
C127	C128	C129	119.8(2)	.	.	.	no
C128	C129	C130	120.5(2)	.	.	.	no
C129	C130	C131	121.7(2)	.	.	.	no
C130	C131	C132	125.38(18)	.	.	.	no
C126	C131	C132	117.30(17)	.	.	.	no
C126	C131	C130	117.10(17)	.	.	.	no
C123	C132	C131	119.18(17)	.	.	.	no
C120	C132	C123	108.68(16)	.	.	.	no
C120	C132	C131	131.92(17)	.	.	.	no
C110	C111	H111	120.3(12)	.	.	.	no
C112	C111	H111	120.5(12)	.	.	.	no
C111	C112	H112	118.6(11)	.	.	.	no
C113	C112	H112	120.8(11)	.	.	.	no
C115	C116	H116	114.1(15)	.	.	.	no
H116'	C116	H116"	106.6(17)	.	.	.	no
C115	C116	H116'	107.7(13)	.	.	.	no
C115	C116	H116"	108.7(12)	.	.	.	no
H116'	C116	H116	109(2)	.	.	.	no
H116"	C116	H116	110.7(19)	.	.	.	no
H117"	C117	H117	110.5(18)	.	.	.	no
H117'	C117	H117"	104.1(17)	.	.	.	no
H117'	C117	H117	109(2)	.	.	.	no
C115	C117	H117'	109.2(13)	.	.	.	no
C115	C117	H117"	113.3(13)	.	.	.	no
C115	C117	H117	110.5(14)	.	.	.	no
H118"	C118	H118	107.8(17)	.	.	.	no
C115	C118	H118	110.7(13)	.	.	.	no
C115	C118	H118'	108.8(13)	.	.	.	no
C115	C118	H118"	111.8(13)	.	.	.	no
H118'	C118	H118"	108.1(19)	.	.	.	no
H118'	C118	H118	109.5(17)	.	.	.	no
O13	C119	H119'	105.2(13)	.	.	.	no
H119"	C119	H119	112(2)	.	.	.	no
O13	C119	H119"	111.9(14)	.	.	.	no
O13	C119	H119	108.2(14)	.	.	.	no
H119'	C119	H119"	108(2)	.	.	.	no
H119'	C119	H119	112(2)	.	.	.	no
C133	C121	H121	107.8(10)	.	.	.	no
C22	C21	C26	121.34(18)	.	.	.	no
C122	C121	H121	109.4(11)	.	.	.	no
C120	C121	H121	113.0(10)	.	.	.	no
N21	C21	C22	120.84(18)	.	.	.	yes
N21	C21	C26	117.72(17)	.	.	.	yes

C121	C122	H122	111.3(12)	.	.	.	no
C123	C122	H122'	110.8(11)	.	.	.	no
C123	C122	H122	115.0(12)	.	.	.	no
H122'	C122	H122	105.3(15)	.	.	.	no
C121	C122	H122'	110.3(11)	.	.	.	no
C21	C22	C23	119.6(2)	.	.	.	no
C22	C23	C24	120.2(2)	.	.	.	no
C123	C124	H124	118.3(13)	.	.	.	no
C125	C124	H124	122.8(13)	.	.	.	no
C23	C24	C25	120.4(2)	.	.	.	no
C124	C125	H125	121.3(11)	.	.	.	no
C24	C25	C26	120.79(19)	.	.	.	no
C126	C125	H125	117.5(11)	.	.	.	no
C21	C26	C27	116.31(16)	.	.	.	no
C25	C26	C27	126.06(17)	.	.	.	no
C21	C26	C25	117.58(18)	.	.	.	no
C126	C127	H127	118.7(13)	.	.	.	no
C128	C127	H127	120.0(14)	.	.	.	no
C28	C27	C220	122.59(17)	.	.	.	no
C26	C27	C28	110.47(16)	.	.	.	no
C26	C27	C220	126.92(17)	.	.	.	no
C129	C128	H128	119.5(14)	.	.	.	no
C127	C128	H128	120.7(14)	.	.	.	no
C29	C28	C213	119.41(17)	.	.	.	no
C27	C28	C213	119.29(17)	.	.	.	no
C27	C28	C29	121.24(17)	.	.	.	no
C28	C29	C210	120.47(18)	.	.	.	no
C130	C129	H129	118.6(12)	.	.	.	no
C128	C129	H129	120.9(12)	.	.	.	no
C129	C130	H130	119.7(12)	.	.	.	no
C131	C130	H130	118.6(12)	.	.	.	no
C121	C133	H133'	109.4(11)	.	.	.	no
C121	C133	H133"	110.5(10)	.	.	.	no
C121	C133	H133	111.8(13)	.	.	.	no
H133'	C133	H133"	110.4(16)	.	.	.	no
H133'	C133	H133	108.3(16)	.	.	.	no
H133"	C133	H133	106.6(17)	.	.	.	no
C21	C22	H22	118.7(12)	.	.	.	no
C23	C22	H22	121.6(12)	.	.	.	no
C24	C23	H23	119.4(12)	.	.	.	no
C22	C23	H23	120.2(12)	.	.	.	no
C25	C24	H24	120.4(11)	.	.	.	no
C23	C24	H24	119.3(11)	.	.	.	no
C24	C25	H25	117.9(12)	.	.	.	no
C26	C25	H25	121.3(12)	.	.	.	no
C28	C29	H29	117.8(13)	.	.	.	no
C210	C29	H29	121.8(13)	.	.	.	no
C29	C210	C211	119.69(19)	.	.	.	no
O23	C210	C29	123.42(18)	.	.	.	yes
O23	C210	C211	116.88(18)	.	.	.	yes
C210	C211	C212	120.5(2)	.	.	.	no
C211	C212	C213	119.7(2)	.	.	.	no
C28	C213	C212	120.18(18)	.	.	.	no
N21	C213	C212	123.69(18)	.	.	.	yes
N21	C213	C28	116.08(16)	.	.	.	yes
O21	C214	O22	125.45(17)	.	.	.	yes
O21	C214	N21	123.90(19)	.	.	.	yes
O22	C214	N21	110.65(17)	.	.	.	yes
O22	C215	C217	109.2(2)	.	.	.	yes
O22	C215	C218	101.6(2)	.	.	.	yes
C216	C215	C217	112.9(2)	.	.	.	no

C216	C215	C218	110.8(2)	.	.	.	no
C217	C215	C218	111.0(2)	.	.	.	no
O22	C215	C216	110.84(18)	.	.	.	yes
C27	C220	C221	126.12(18)	.	.	.	no
C221	C220	C232	105.72(16)	.	.	.	no
C27	C220	C232	127.86(17)	.	.	.	no
C222	C221	C233	111.64(17)	.	.	.	no
C220	C221	C222	102.88(16)	.	.	.	no
C220	C221	C233	112.97(16)	.	.	.	no
C221	C222	C223	103.94(17)	.	.	.	no
C222	C223	C224	127.16(19)	.	.	.	no
C222	C223	C232	111.43(18)	.	.	.	no
C224	C223	C232	121.42(19)	.	.	.	no
C223	C224	C225	118.8(2)	.	.	.	no
C224	C225	C226	122.0(2)	.	.	.	no
C225	C226	C231	119.26(18)	.	.	.	no
C225	C226	C227	121.0(2)	.	.	.	no
C227	C226	C231	119.72(18)	.	.	.	no
C226	C227	C228	121.4(2)	.	.	.	no
C227	C228	C229	119.5(2)	.	.	.	no
C228	C229	C230	120.7(2)	.	.	.	no
C229	C230	C231	121.47(19)	.	.	.	no
C230	C231	C232	124.98(19)	.	.	.	no
C226	C231	C232	117.81(17)	.	.	.	no
C226	C231	C230	117.12(17)	.	.	.	no
C220	C232	C223	108.22(16)	.	.	.	no
C220	C232	C231	131.83(17)	.	.	.	no
C223	C232	C231	119.84(19)	.	.	.	no
C210	C211	H211	117.8(11)	.	.	.	no
C212	C211	H211	121.7(12)	.	.	.	no
C211	C212	H212	120.8(13)	.	.	.	no
C213	C212	H212	119.4(13)	.	.	.	no
C215	C216	H216'	109.3(15)	.	.	.	no
C215	C216	H216"	112.4(15)	.	.	.	no
C215	C216	H216	114.1(15)	.	.	.	no
H216'	C216	H216"	106(2)	.	.	.	no
H216'	C216	H216	107(2)	.	.	.	no
H216"	C216	H216	107(2)	.	.	.	no
C215	C217	H217'	109.4(12)	.	.	.	no
C215	C217	H217"	109.2(15)	.	.	.	no
C215	C217	H217	109.7(14)	.	.	.	no
H217'	C217	H217"	104.0(19)	.	.	.	no
H217'	C217	H217	109.1(19)	.	.	.	no
H217"	C217	H217	115(2)	.	.	.	no
C215	C218	H218'	109.2(14)	.	.	.	no
C215	C218	H218"	112(2)	.	.	.	no
C215	C218	H218	110.1(15)	.	.	.	no
H218'	C218	H218"	110(3)	.	.	.	no
H218'	C218	H218	108(2)	.	.	.	no
H218"	C218	H218	108(3)	.	.	.	no
O23	C219	H219'	106.8(12)	.	.	.	no
O23	C219	H219"	110.6(12)	.	.	.	no
O23	C219	H219	109.7(14)	.	.	.	no
H219'	C219	H219"	110.4(17)	.	.	.	no
H219'	C219	H219	109.0(18)	.	.	.	no
H219"	C219	H219	110.3(19)	.	.	.	no
C220	C221	H221	110.8(13)	.	.	.	no
C222	C221	H221	109.2(12)	.	.	.	no
C233	C221	H221	109.2(12)	.	.	.	no
C221	C222	H222'	112.2(11)	.	.	.	no
C221	C222	H222	111.0(11)	.	.	.	no

C223	C222	H222'	110.8(11)	.	.	.	.	no
C223	C222	H222	112.2(11)	.	.	.	.	no
H222'	C222	H222	106.8(15)	.	.	.	.	no
C223	C224	H224	119.1(11)	.	.	.	.	no
C225	C224	H224	122.0(11)	.	.	.	.	no
C224	C225	H225	118.2(12)	.	.	.	.	no
C226	C225	H225	119.7(12)	.	.	.	.	no
C226	C227	H227	118.4(12)	.	.	.	.	no
C228	C227	H227	120.2(12)	.	.	.	.	no
C227	C228	H228	118.7(13)	.	.	.	.	no
C229	C228	H228	121.7(13)	.	.	.	.	no
C228	C229	H229	118.3(12)	.	.	.	.	no
C230	C229	H229	121.0(12)	.	.	.	.	no
C229	C230	H230	120.7(11)	.	.	.	.	no
C231	C230	H230	117.8(11)	.	.	.	.	no
C221	C233	H233'	109.7(11)	.	.	.	.	no
C221	C233	H233"	111.9(14)	.	.	.	.	no
C221	C233	H233	111.1(13)	.	.	.	.	no
H233'	C233	H233"	106.0(17)	.	.	.	.	no
H233'	C233	H233	109.9(16)	.	.	.	.	no
H233"	C233	H233	108(2)	.	.	.	.	no

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C115	O12	C114	O11	-14.6(3)	.	.	.	.	no
C115	O12	C114	N11	166.91(15)	.	.	.	.	no
C114	O12	C115	C116	61.6(2)	.	.	.	.	no
C114	O12	C115	C117	-62.3(2)	.	.	.	.	no
C114	O12	C115	C118	-179.91(16)	.	.	.	.	no
C119	O13	C110	C19	-166.39(18)	.	.	.	.	no
C119	O13	C110	C111	14.7(3)	.	.	.	.	no
C215	O22	C214	N21	169.67(17)	.	.	.	.	no
C214	O22	C215	C216	64.2(2)	.	.	.	.	no
C214	O22	C215	C217	-60.8(2)	.	.	.	.	no
C214	O22	C215	C218	-178.0(2)	.	.	.	.	no
C215	O22	C214	O21	-10.6(3)	.	.	.	.	no
C219	O23	C210	C29	-7.6(3)	.	.	.	.	no
C219	O23	C210	C211	171.2(2)	.	.	.	.	no
C113	N11	C11	C12	-139.35(19)	.	.	.	.	no
C113	N11	C11	C16	37.2(2)	.	.	.	.	no
C114	N11	C11	C12	44.8(3)	.	.	.	.	no
C114	N11	C11	C16	-138.69(18)	.	.	.	.	no
C11	N11	C113	C18	-39.9(2)	.	.	.	.	no
C11	N11	C113	C112	137.06(19)	.	.	.	.	no
C11	N11	C114	O11	-12.5(3)	.	.	.	.	no
C114	N11	C113	C18	135.83(19)	.	.	.	.	no
C114	N11	C113	C112	-47.2(3)	.	.	.	.	no
C113	N11	C114	O12	-9.4(2)	.	.	.	.	no
C11	N11	C114	O12	166.07(15)	.	.	.	.	no
C113	N11	C114	O11	172.06(18)	.	.	.	.	no
C213	N21	C21	C22	-139.9(2)	.	.	.	.	no
C214	N21	C213	C212	-52.5(3)	.	.	.	.	no

C213	N21	C21	C26	36.6(2)	.	.	.	no
C214	N21	C21	C22	50.8(3)	.	.	.	no
C214	N21	C21	C26	-132.84(19)	.	.	.	no
C21	N21	C213	C28	-38.6(2)	.	.	.	no
C21	N21	C213	C212	138.7(2)	.	.	.	no
C214	N21	C213	C28	130.2(2)	.	.	.	no
C21	N21	C214	O22	170.81(16)	.	.	.	no
C213	N21	C214	O21	-177.28(19)	.	.	.	no
C21	N21	C214	O21	-9.0(3)	.	.	.	no
C213	N21	C214	O22	2.5(3)	.	.	.	no
N11	C11	C12	C13	174.9(2)	.	.	.	no
C16	C11	C12	C13	-1.5(3)	.	.	.	no
N11	C11	C16	C15	-171.80(18)	.	.	.	no
N11	C11	C16	C17	5.8(2)	.	.	.	no
C12	C11	C16	C15	4.8(3)	.	.	.	no
C12	C11	C16	C17	-177.64(18)	.	.	.	no
C11	C12	C13	C14	-2.4(4)	.	.	.	no
C12	C13	C14	C15	3.1(4)	.	.	.	no
C13	C14	C15	C16	0.3(4)	.	.	.	no
C14	C15	C16	C17	178.5(2)	.	.	.	no
C14	C15	C16	C11	-4.1(3)	.	.	.	no
C11	C16	C17	C120	131.4(2)	.	.	.	no
C15	C16	C17	C18	133.2(2)	.	.	.	no
C11	C16	C17	C18	-44.2(2)	.	.	.	no
C15	C16	C17	C120	-51.3(3)	.	.	.	no
C18	C17	C120	C121	-169.08(17)	.	.	.	no
C16	C17	C120	C121	16.0(3)	.	.	.	no
C120	C17	C18	C113	-133.6(2)	.	.	.	no
C16	C17	C18	C19	-133.95(19)	.	.	.	no
C16	C17	C120	C132	-169.60(18)	.	.	.	no
C18	C17	C120	C132	5.4(3)	.	.	.	no
C120	C17	C18	C19	50.5(3)	.	.	.	no
C16	C17	C18	C113	42.0(2)	.	.	.	no
C17	C18	C113	C112	-178.05(17)	.	.	.	no
C113	C18	C19	C110	2.2(3)	.	.	.	no
C19	C18	C113	N11	175.09(17)	.	.	.	no
C19	C18	C113	C112	-1.9(3)	.	.	.	no
C17	C18	C19	C110	178.09(18)	.	.	.	no
C17	C18	C113	N11	-1.0(2)	.	.	.	no
C18	C19	C110	O13	-179.19(17)	.	.	.	no
C18	C19	C110	C111	-0.3(3)	.	.	.	no
N21	C21	C22	C23	175.6(2)	.	.	.	no
C26	C21	C22	C23	-0.6(3)	.	.	.	no
N21	C21	C26	C25	-173.16(17)	.	.	.	no
N21	C21	C26	C27	4.5(2)	.	.	.	no
C22	C21	C26	C25	3.2(3)	.	.	.	no
C22	C21	C26	C27	-179.07(19)	.	.	.	no
C21	C22	C23	C24	-1.5(4)	.	.	.	no
C22	C23	C24	C25	1.0(4)	.	.	.	no
C23	C24	C25	C26	1.7(3)	.	.	.	no
C24	C25	C26	C21	-3.8(3)	.	.	.	no
C24	C25	C26	C27	178.80(19)	.	.	.	no
C21	C26	C27	C28	-41.0(2)	.	.	.	no
C21	C26	C27	C220	137.5(2)	.	.	.	no
C25	C26	C27	C28	136.46(19)	.	.	.	no
C25	C26	C27	C220	-45.0(3)	.	.	.	no
C26	C27	C28	C29	-137.39(18)	.	.	.	no
C26	C27	C28	C213	39.6(2)	.	.	.	no
C220	C27	C28	C29	44.0(3)	.	.	.	no
C220	C27	C28	C213	-138.94(19)	.	.	.	no
C26	C27	C220	C232	-169.84(18)	.	.	.	no

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 C28     C27     C220    C232         8.5(3)     .       .       .       no
 C26     C27     C220    C221        17.4(3)     .       .       .       no
 C28     C27     C220    C221    -164.28(17)     .       .       .       no
 C27     C28     C213    N21          -0.4(3)    .       .       .       no
 C29     C28     C213    C212         -0.7(3)    .       .       .       no
 C29     C28     C213    N21       176.64(17)    .       .       .       no
 C27     C28     C213    C212    -177.82(19)     .       .       .       no
 C27     C28     C29     C210      179.59(18)    .       .       .       no
 C213    C28     C29     C210         2.6(3)     .       .       .       no
 C28     C29     C210    C211        -2.2(3)     .       .       .       no
 C28     C29     C210    O23       176.56(18)    .       .       .       no
 O23     C210    C211    C212      -178.8(2)     .       .       .       no
 C29     C210    C211    C212         0.1(3)     .       .       .       no
 C210    C211    C212    C213         1.8(4)     .       .       .       no
 C211    C212    C213    N21       -178.6(2)     .       .       .       no
 C211    C212    C213    C28          -1.4(3)    .       .       .       no
 C27     C220    C221    C222       146.2(2)     .       .       .       no
 C27     C220    C221    C233       -93.3(2)     .       .       .       no
 C232    C220    C221    C222     -27.92(19)     .       .       .       no
 C232    C220    C221    C233        92.6(2)     .       .       .       no
 C27     C220    C232    C223    -152.17(19)     .       .       .       no
 C27     C220    C232    C231        31.8(3)     .       .       .       no
 C221    C220    C232    C223        21.8(2)     .       .       .       no
 C221    C220    C232    C231    -154.28(19)     .       .       .       no
 C220    C221    C222    C223        23.9(2)     .       .       .       no
 C233    C221    C222    C223       -97.5(2)     .       .       .       no
 C221    C222    C223    C224       168.4(2)     .       .       .       no
 C221    C222    C223    C232       -11.8(2)     .       .       .       no
 C222    C223    C224    C225      -177.9(2)     .       .       .       no
 C232    C223    C224    C225         2.4(3)     .       .       .       no
 C222    C223    C232    C220        -6.1(2)     .       .       .       no
 C222    C223    C232    C231      170.55(18)    .       .       .       no
 C224    C223    C232    C220      173.74(19)    .       .       .       no
 C224    C223    C232    C231        -9.7(3)     .       .       .       no
 C223    C224    C225    C226         4.5(4)     .       .       .       no
 C224    C225    C226    C227       173.9(2)     .       .       .       no
 C224    C225    C226    C231        -3.9(3)     .       .       .       no
 C225    C226    C227    C228      -175.1(2)     .       .       .       no
 C231    C226    C227    C228         2.7(3)     .       .       .       no
 C225    C226    C231    C230      173.44(19)    .       .       .       no
 C225    C226    C231    C232        -3.3(3)     .       .       .       no
 C227    C226    C231    C230        -4.4(3)     .       .       .       no
 C227    C226    C231    C232      178.89(19)    .       .       .       no
 C226    C227    C228    C229         0.5(4)     .       .       .       no
 C227    C228    C229    C230        -1.9(3)     .       .       .       no
 C228    C229    C230    C231         0.1(3)     .       .       .       no
 C229    C230    C231    C226         3.0(3)     .       .       .       no
 C229    C230    C231    C232      179.52(18)    .       .       .       no
 C226    C231    C232    C220    -174.42(19)     .       .       .       no
 C226    C231    C232    C223         9.9(3)     .       .       .       no
 C230    C231    C232    C220         9.1(3)     .       .       .       no
 C230    C231    C232    C223    -166.55(18)     .       .       .       no

loop_
_geom_contact_atom_site_label_1
_geom_contact_atom_site_label_2
_geom_contact_distance
_geom_contact_site_symmetry_1
_geom_contact_site_symmetry_2
_geom_contact_publ_flag
 O11     C12        2.854(3)                    .       .                   no
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O11	C116	2.933(3)	.	.	no
O11	C117	3.087(3)	.	.	no
O11	C224	3.333(3)	.	.	no
O11	O11	3.225(2)	.	3_656	no
O11	C117	3.410(3)	.	3_656	no
O12	C112	2.828(2)	.	.	no
O13	C125	3.306(3)	.	3_566	no
O21	C219	3.240(3)	.	2_655	no
O21	C22	2.873(3)	.	.	no
O21	C217	3.024(3)	.	.	no
O21	C216	2.957(3)	.	.	no
O22	C212	2.843(3)	.	.	no
O11	H116	2.45(3)	.	.	no
O11	H117"	2.59(2)	.	.	no
O11	H224	2.43(2)	.	.	no
O11	H12	2.375(19)	.	.	no
O11	H117"	2.55(2)	.	3_656	no
O12	H112	2.571(18)	.	.	no
O12	H222	2.71(2)	.	.	no
O13	H24	2.759(19)	.	3_566	no
O13	H125	2.42(2)	.	3_566	no
O21	H217"	2.45(3)	.	.	no
O21	H124	2.59(2)	.	1_655	no
O21	H216	2.44(3)	.	.	no
O21	H22	2.504(19)	.	.	no
O21	H219'	2.39(2)	.	2_655	no
O22	H212	2.523(19)	.	.	no
O23	H111	2.57(2)	.	4_554	no
C12	O11	2.854(3)	.	.	no
C12	C12	3.286(3)	.	3_556	no
C15	C121	3.217(3)	.	.	no
C17	C130	3.442(3)	.	.	no
C18	C130	3.037(3)	.	.	no
C18	C131	3.355(3)	.	.	no
C19	C132	3.331(3)	.	.	no
C19	C130	3.181(3)	.	.	no
C19	C131	3.322(3)	.	.	no
C22	O21	2.873(3)	.	.	no
C22	C228	3.478(3)	.	2_655	no
C24	C128	3.572(4)	.	3_666	no
C24	C119	3.548(4)	.	3_566	no
C25	C221	3.247(3)	.	.	no
C27	C230	3.417(3)	.	.	no
C28	C230	3.003(3)	.	.	no
C28	C231	3.278(3)	.	.	no
C29	C230	3.125(3)	.	.	no
C29	C231	3.137(3)	.	.	no
C29	C232	3.131(3)	.	.	no
C112	O12	2.828(2)	.	.	no
C113	C130	3.516(3)	.	.	no
C14	H217'	3.09(2)	.	2_645	no
C114	C222	3.523(3)	.	.	no
C15	H121	2.592(19)	.	.	no
C16	H121	2.908(18)	.	.	no
C116	O11	2.933(3)	.	.	no
C17	H222'	2.926(18)	.	.	no
C17	H130	2.87(2)	.	.	no
C17	H233	3.05(3)	.	1_455	no
C117	O11	3.087(3)	.	.	no
C117	O11	3.410(3)	.	3_656	no
C18	H130	2.43(2)	.	.	no

C18	H116'	3.04(2)	.	1_455	no
C119	C24	3.548(4)	.	3_566	no
C119	C125	3.598(3)	.	3_566	no
C19	H130	2.938(19)	.	.	no
C119	C219	3.511(4)	.	4_555	no
C121	C230	3.509(3)	.	1_455	no
C121	C15	3.217(3)	.	.	no
C122	C230	3.529(3)	.	1_455	no
C122	C233	3.562(4)	.	1_455	no
C23	H119'	3.06(3)	.	3_566	no
C24	H119'	2.71(3)	.	3_566	no
C24	H128	2.85(2)	.	3_666	no
C25	H221	2.65(2)	.	.	no
C125	C119	3.598(3)	.	3_566	no
C25	H128	3.04(2)	.	3_666	no
C125	C127	3.360(4)	.	3_566	no
C125	O13	3.306(3)	.	3_566	no
C26	H221	2.96(2)	.	.	no
C126	C126	3.520(3)	.	3_566	no
C126	C127	3.563(3)	.	3_566	no
C27	H230	2.841(18)	.	.	no
C127	C125	3.360(4)	.	3_566	no
C27	H122'	2.903(18)	.	1_655	no
C127	C126	3.563(3)	.	3_566	no
C128	C24	3.572(4)	.	3_666	no
C28	H230	2.462(18)	.	.	no
C29	H230	2.996(18)	.	.	no
C29	H219"	2.82(2)	.	.	no
C29	H219	2.62(2)	.	.	no
C29	H216"	3.07(3)	.	1_455	no
C130	C113	3.516(3)	.	.	no
C130	C222	3.541(3)	.	.	no
C130	C18	3.037(3)	.	.	no
C130	C17	3.442(3)	.	.	no
C130	C221	3.489(3)	.	.	no
C130	C19	3.181(3)	.	.	no
C131	C18	3.355(3)	.	.	no
C131	C19	3.322(3)	.	.	no
C132	C19	3.331(3)	.	.	no
C133	C222	3.590(4)	.	.	no
C110	H118'	2.98(3)	.	1_455	no
C110	H125	3.07(2)	.	3_566	no
C111	H119	2.77(3)	.	.	no
C111	H119"	2.76(2)	.	.	no
C212	O22	2.843(3)	.	.	no
C112	H13	2.83(2)	.	3_556	no
C113	H130	2.69(2)	.	.	no
C213	C230	3.472(3)	.	.	no
C114	H117"	2.81(2)	.	.	no
C114	H224	3.06(2)	.	.	no
C114	H222	2.81(2)	.	.	no
C114	H12	2.78(2)	.	.	no
C114	H116	2.94(3)	.	.	no
C114	H112	2.938(18)	.	.	no
C116	H12	3.00(2)	.	3_656	no
C216	O21	2.957(3)	.	.	no
C117	H225	3.01(2)	.	3_656	no
C217	O21	3.024(3)	.	.	no
C119	H125	2.924(19)	.	3_566	no
C119	H219'	2.81(2)	.	4_555	no
C119	H111	2.50(2)	.	.	no

C219	C119	3.511(4)	.	4_554	no
C219	O21	3.240(3)	.	2_645	no
C120	H130	2.97(2)	.	.	no
C120	H233	2.84(3)	.	1_455	no
C120	H222'	2.764(18)	.	.	no
C120	H19	3.040(18)	.	.	no
C221	C130	3.489(3)	.	.	no
C121	H15	2.89(2)	.	.	no
C221	C25	3.247(3)	.	.	no
C122	H230	2.948(18)	.	1_455	no
C222	C130	3.541(3)	.	.	no
C222	C114	3.523(3)	.	.	no
C222	C133	3.590(4)	.	.	no
C123	H133	3.10(2)	.	.	no
C123	H233"	3.07(3)	.	1_455	no
C224	O11	3.333(3)	.	.	no
C125	H24	3.097(18)	.	.	no
C125	H25	3.037(19)	.	.	no
C126	H25	2.84(2)	.	.	no
C228	C22	3.478(3)	.	2_645	no
C230	C27	3.417(3)	.	.	no
C230	C121	3.509(3)	.	1_655	no
C230	C28	3.003(3)	.	.	no
C130	H221	2.84(2)	.	.	no
C230	C213	3.472(3)	.	.	no
C230	C122	3.529(3)	.	1_655	no
C230	C29	3.125(3)	.	.	no
C131	H25	3.04(2)	.	.	no
C131	H221	2.945(19)	.	.	no
C231	C29	3.137(3)	.	.	no
C231	C28	3.278(3)	.	.	no
C132	H133	3.05(2)	.	.	no
C132	H19	3.024(18)	.	.	no
C232	C29	3.131(3)	.	.	no
C233	C122	3.562(4)	.	1_655	no
C133	H29	2.99(2)	.	.	no
C133	H222'	2.864(18)	.	.	no
C212	H227	2.99(2)	.	2_655	no
C213	H230	2.733(19)	.	.	no
C214	H212	3.00(2)	.	.	no
C214	H217"	2.79(3)	.	.	no
C214	H216	2.90(3)	.	.	no
C214	H122	3.05(2)	.	1_655	no
C214	H22	2.82(2)	.	.	no
C219	H29	2.49(2)	.	.	no
C219	H22	2.95(2)	.	2_645	no
C219	H119"	2.98(2)	.	4_554	no
C219	H217"	3.00(3)	.	2_645	no
C220	H133	2.92(3)	.	.	no
C220	H122'	2.732(18)	.	1_655	no
C220	H230	2.954(18)	.	.	no
C220	H29	2.83(2)	.	.	no
C221	H25	2.818(19)	.	.	no
C222	H130	3.02(2)	.	.	no
C222	H133	3.06(2)	.	.	no
C223	H233	3.07(2)	.	.	no
C225	H15	3.062(19)	.	1_655	no
C225	H14	2.937(19)	.	1_655	no
C226	H15	3.03(2)	.	1_655	no
C230	H121	2.845(18)	.	1_655	no
C231	H29	2.961(19)	.	.	no

C231	H121	2.884(18)	.	1_655	no
C231	H15	3.10(2)	.	1_655	no
C232	H29	2.74(2)	.	.	no
C232	H233	3.05(2)	.	.	no
C233	H19	3.068(18)	.	1_655	no
C233	H122'	2.869(18)	.	1_655	no
H116'	C18	3.04(2)	.	1_655	no
H116'	H118'	2.49(3)	.	.	no
H116"	H222	2.40(3)	.	.	no
H116"	H118	2.49(3)	.	.	no
H117'	H118'	2.56(3)	.	.	no
H117"	C114	2.81(2)	.	.	no
H117"	O11	2.59(2)	.	.	no
H117"	O11	2.55(2)	.	3_656	no
H117"	H224	2.54(3)	.	3_656	no
H117"	H116	2.57(3)	.	.	no
H118'	C110	2.98(3)	.	1_655	no
H118'	H117'	2.56(3)	.	.	no
H118'	H116'	2.49(3)	.	.	no
H118"	H117	2.53(3)	.	.	no
H118"	H211	2.43(3)	.	4_555	no
H119'	C24	2.71(3)	.	3_566	no
H119'	H24	2.56(3)	.	3_566	no
H119'	C23	3.06(3)	.	3_566	no
H119"	H111	2.36(3)	.	.	no
H119"	C111	2.76(2)	.	.	no
H119"	C219	2.98(2)	.	4_555	no
H119"	H219'	2.19(3)	.	4_555	no
H122'	C27	2.903(18)	.	1_455	no
H122'	C220	2.732(18)	.	1_455	no
H122'	C233	2.869(18)	.	1_455	no
H122'	H233"	2.48(3)	.	1_455	no
H122'	H230	2.57(3)	.	1_455	no
H133'	H219"	2.45(3)	.	.	no
H133'	H122	2.45(3)	.	.	no
H133"	H222'	2.50(3)	.	.	no
H12	C114	2.78(2)	.	.	no
H12	C116	3.00(2)	.	3_656	no
H12	H116	2.55(3)	.	3_656	no
H12	O11	2.375(19)	.	.	no
H216'	H218'	2.52(3)	.	.	no
H13	C112	2.83(2)	.	3_556	no
H216"	C29	3.07(3)	.	1_655	no
H216"	H218	2.51(4)	.	.	no
H216"	H122	2.54(3)	.	1_655	no
H14	C225	2.937(19)	.	1_455	no
H217'	H218'	2.57(3)	.	.	no
H217'	C14	3.09(2)	.	2_655	no
H15	C225	3.062(19)	.	1_455	no
H15	C121	2.89(2)	.	.	no
H15	H121	2.06(3)	.	.	no
H15	C226	3.03(2)	.	1_455	no
H15	C231	3.10(2)	.	1_455	no
H217"	O21	2.45(3)	.	.	no
H217"	C219	3.00(3)	.	2_655	no
H217"	H216	2.52(4)	.	.	no
H217"	C214	2.79(3)	.	.	no
H218'	H217'	2.57(3)	.	.	no
H218'	H216'	2.52(3)	.	.	no
H218"	H217	2.51(4)	.	.	no
H219'	C119	2.81(2)	.	4_554	no

H219'	O21	2.39(2)	.	2_645	no
H219'	H119"	2.19(3)	.	4_554	no
H19	C120	3.040(18)	.	.	no
H19	C132	3.024(18)	.	.	no
H19	C233	3.068(18)	.	1_455	no
H219"	C29	2.82(2)	.	.	no
H219"	H133'	2.45(3)	.	.	no
H219"	H29	2.35(3)	.	.	no
H222'	C120	2.764(18)	.	.	no
H222'	C133	2.864(18)	.	.	no
H222'	C17	2.926(18)	.	.	no
H222'	H133"	2.50(3)	.	.	no
H222'	H133	2.51(3)	.	.	no
H233'	H222	2.51(3)	.	.	no
H22	C219	2.95(2)	.	2_655	no
H22	C214	2.82(2)	.	.	no
H22	O21	2.504(19)	.	.	no
H233"	C123	3.07(3)	.	1_655	no
H233"	H122'	2.48(3)	.	1_655	no
H24	C125	3.097(18)	.	.	no
H24	O13	2.759(19)	.	3_566	no
H24	H119'	2.56(3)	.	3_566	no
H25	H221	2.02(3)	.	.	no
H25	C125	3.037(19)	.	.	no
H25	C126	2.84(2)	.	.	no
H25	C131	3.04(2)	.	.	no
H25	C221	2.818(19)	.	.	no
H29	C231	2.961(19)	.	.	no
H29	C232	2.74(2)	.	.	no
H29	H219"	2.35(3)	.	.	no
H29	H133	2.53(3)	.	.	no
H29	H219	2.24(3)	.	.	no
H29	C133	2.99(2)	.	.	no
H29	C219	2.49(2)	.	.	no
H29	C220	2.83(2)	.	.	no
H111	C119	2.50(2)	.	.	no
H111	H119"	2.36(3)	.	.	no
H111	H119	2.26(3)	.	.	no
H111	O23	2.57(2)	.	4_555	no
H112	C114	2.938(18)	.	.	no
H112	O12	2.571(18)	.	.	no
H116	C114	2.94(3)	.	.	no
H116	H117"	2.57(3)	.	.	no
H116	O11	2.45(3)	.	.	no
H116	H12	2.55(3)	.	3_656	no
H117	H118"	2.53(3)	.	.	no
H117	H225	2.58(3)	.	3_656	no
H118	H116"	2.49(3)	.	.	no
H119	H111	2.26(3)	.	.	no
H119	C111	2.77(3)	.	.	no
H121	H15	2.06(3)	.	.	no
H121	C15	2.592(19)	.	.	no
H121	C16	2.908(18)	.	.	no
H121	C230	2.845(18)	.	1_455	no
H121	C231	2.884(18)	.	1_455	no
H122	H133'	2.45(3)	.	.	no
H122	H216"	2.54(3)	.	1_455	no
H122	C214	3.05(2)	.	1_455	no
H124	O21	2.59(2)	.	1_455	no
H125	H127	2.40(3)	.	.	no
H125	C110	3.07(2)	.	3_566	no

H125	C119	2.924(19)	.	3_566	no
H125	O13	2.42(2)	.	3_566	no
H127	H125	2.40(3)	.	.	no
H128	C24	2.85(2)	.	3_666	no
H128	C25	3.04(2)	.	3_666	no
H130	C17	2.87(2)	.	.	no
H130	C18	2.43(2)	.	.	no
H130	C19	2.938(19)	.	.	no
H130	C113	2.69(2)	.	.	no
H130	C222	3.02(2)	.	.	no
H130	C120	2.97(2)	.	.	no
H133	C132	3.05(2)	.	.	no
H133	C220	2.92(3)	.	.	no
H133	C123	3.10(2)	.	.	no
H133	H222'	2.51(3)	.	.	no
H133	H29	2.53(3)	.	.	no
H133	C222	3.06(2)	.	.	no
H211	H118"	2.43(3)	.	4_554	no
H212	O22	2.523(19)	.	.	no
H212	C214	3.00(2)	.	.	no
H212	H225	2.55(3)	.	2_655	no
H216	O21	2.44(3)	.	.	no
H216	C214	2.90(3)	.	.	no
H216	H217"	2.52(4)	.	.	no
H217	H218"	2.51(4)	.	.	no
H218	H216"	2.51(4)	.	.	no
H219	C29	2.62(2)	.	.	no
H219	H29	2.24(3)	.	.	no
H221	C25	2.65(2)	.	.	no
H221	C26	2.96(2)	.	.	no
H221	C130	2.84(2)	.	.	no
H221	C131	2.945(19)	.	.	no
H221	H25	2.02(3)	.	.	no
H222	O12	2.71(2)	.	.	no
H222	C114	2.81(2)	.	.	no
H222	H116"	2.40(3)	.	.	no
H222	H233'	2.51(3)	.	.	no
H224	O11	2.43(2)	.	.	no
H224	C114	3.06(2)	.	.	no
H224	H117"	2.54(3)	.	3_656	no
H225	H227	2.45(3)	.	.	no
H225	H212	2.55(3)	.	2_645	no
H225	C117	3.01(2)	.	3_656	no
H225	H117	2.58(3)	.	3_656	no
H227	H225	2.45(3)	.	.	no
H227	C212	2.99(2)	.	2_645	no
H230	C27	2.841(18)	.	.	no
H230	C28	2.462(18)	.	.	no
H230	C29	2.996(18)	.	.	no
H230	C122	2.948(18)	.	1_655	no
H230	C213	2.733(19)	.	.	no
H230	C220	2.954(18)	.	.	no
H230	H122'	2.57(3)	.	1_655	no
H233	C17	3.05(3)	.	1_655	no
H233	C120	2.84(3)	.	1_655	no
H233	C223	3.07(2)	.	.	no
H233	C232	3.05(2)	.	.	no

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loop_
_geom_hbond_atom_site_label_D
_geom_hbond_atom_site_label_H
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_geom_hbond_distance_DH
_geom_hbond_distance_HA
_geom_hbond_distance_DA
_geom_hbond_angle_DHA
_geom_hbond_site_symmetry_A
_geom_hbond_publ_flag
#
#D   H   A   D - H  H...A   D...A    D - H...A  symm(A)
#
C117    H117"   O11        0.98(2)    2.59(2)   3.087(3)  111.7(15)     .   yes
C117    H117"   O11        0.98(2)    2.55(2)   3.410(3)  147.5(15)   3_656 yes
C12     H12     O11      0.942(19)  2.375(19)   2.854(3)  111.1(15)     .   yes
C217    H217"   O21        1.04(3)    2.45(3)   3.024(3)  113.4(18)     .   yes
C219    H219'   O21        1.03(2)    2.39(2)   3.240(3)  138.8(16)   2_645 yes
C22     H22     O21        0.96(2)  2.504(19)   2.873(3)  103.0(14)     .   yes
C111    H111    O23        0.98(2)    2.57(2)   3.491(3)  156.0(14)   4_555 yes
C116    H116    O11        1.00(2)    2.45(3)   2.933(3)  109.5(18)     .   yes
C124    H124    O21        0.94(2)    2.59(2)   3.473(3)  155.6(17)   1_455 yes
C125    H125    O13        0.98(2)    2.42(2)   3.306(3)  150.4(15)   3_566 yes
C216    H216    O21        1.00(2)    2.44(3)   2.957(3)  111.5(19)     .   yes
C224    H224    O11        1.00(2)    2.43(2)   3.333(3)  150.5(15)     .   yes

#===END of Crystallographic Information File
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